Low-energy muon-transfer reaction from hydrogen isotopes to helium isotopes

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Direct muon transfer in low-energy collisions of the muonic hydrogen H_μ and helium (He^{++}) is considered in a three-body quantum-mechanical framework of coordinate-space integro-differential Faddeev-Hahn-type equations within two- and six-state close coupling approximations. The final-state Coulomb interaction is treated without any approximation employing appropriate Coulomb waves in the final state. The present results agree reasonably well with previous semiclassical calculations.
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Experimental investigation of the low-energy muon transfer in collision of muonic hydrogen H_μ (bound state of a hydrogen isotope and muon μ^-) and He is important for muon catalyzed fusion cycle of hydrogen isotopes [1]. If the hydrogen is contaminated by He, then the muon-catalyzed fusion of hydrogen isotopes will be affected by muon transfer from H_μ to He. This makes the study of muon transfer from H_μ to He of special relevance. The study of such collisions involving three charged particles is also interesting from a theoretical point of view as an example of rearrangement scattering with Coulomb interaction in the final state. Such reactions with post-collision Coulomb interaction between clusters appear frequently in atomic and molecular physics.

Recently, we formulated [2] a few-body quantum-mechanical description of direct muon-transfer reaction from H_μ to different nuclei using the Faddeev-Hahn-type few-body equations [3, 4] in the close-coupling approximation. We applied this formulation successfully to the study of muon transfer among various hydrogen isotopes. In that study there was no final-state Coulomb interaction. Later on we extended this approach to the study of muon transfer from hydrogen isotopes to He and Li, where the final-state Coulomb interaction is appropriately included in the calculational scheme [5]. Next we included heavier targets such as, C, O [5, 6], Ne, S, and Ar [7], in the scheme, where appropriate polarization potentials were included in addition to the final-state Coulomb interaction. In case of these heavy targets the muon transfer rates from H_μ agree well with the existing experimental results [5, 6, 7]. In case of these heavier targets there is evidence [7, 8] that the muon is absorbed in a specific final state of the heavy nuclei, and hence, the muon-transfer rates were calculated in a two-state close-coupling approximation including a single state each of the target and the incident H_μ.

In this report, we perform a two- and six-state calculation of direct muon-transfer from H_μ to He isotopes and compare with other calculations. The reaction we study is

$$(H_\mu)_{1s} + He^{++} \to (He_\mu)^+_{1s} + H^+, \qquad (0.1)$$

where He^{++} represents the He nucleus and $(He_\mu)^+_{1s}$ the hydrogen-like bound state of He^{++} and a muon. The present study is meant to test the accuracy and the convergence trend of our approach. For the lighter target such as He, muon transfer could take place via direct as well as compound molecular formation. The experimental rates include the molecular formation [9]. The method we consider here is not applicable to muon transfer via molecular formation. The experimental transfer rates via molecular formation leads to much higher results in the case of target He while compared to the theoretical result of direct muon transfer. For heavier targets, such as C, O, Ne, Ar etc., the molecular rates are highly suppressed and the muon transfer takes place essentially via the direct channel and our theoretical direct rates are in agreement with experiment [5, 6, 7].

For the theoretical treatment of a three-body muon-transfer rearrangement process, Faddeev-type equations [3], especially the modified version proposed by Hahn [4], appear to be very suitable. The two possible asymptotic two-cluster configurations of the above rearrangement problem are conveniently tackled by a set of two coupled Faddeev-Hahn-type equations for components Ψ_1 and Ψ_2 of the wave function $\Psi = \Psi_1 + \Psi_2$, where each component carrys the asymptotic boundary condition for a specific configuration [10]. These equations are very useful to incorporate distortion potentials for specific initial and final asymptotic states [11]. It is possible to include the final-state Coulomb interaction explicitly in these equations, so that a low-order approximation to these equations produces the correct asymptotic behavior [11].

Here we quote the Faddeev-Hahn-type two-component equations used in the close coupling type approximation for the calculation of muon transfer rates [2, 6]. We denote He^{++} by 1, the hydrogen isotope(s) by 2 and muon by 3. Below the three-body breakup threshold, following two-cluster asymptotic configurations are possible in the system 123: (23) $-$ 1 and (13) $-$ 2. These two configurations correspond to two distinct physical channels, denoted by 1 and 2, respectively. These configurations are determined by the Jacobi coordinates $(\vec{r}_{j3}, \vec{\rho}_k)$: $\vec{r}_{13} = \vec{r}_3 - \vec{r}_1$, $\vec{\rho}_2 = (\vec{r}_3 + m_1\vec{r}_1)/(1+m_1) - \vec{r}_2$, $\vec{r}_{23} = \vec{r}_3 - \vec{r}_2$, $\vec{\rho}_1 = (\vec{r}_3 + m_2\vec{r}_2)/(1+m_2) - \vec{r}_1$, where $\vec{r}_i$, m_i $(i = 1, 2, 3,)$ are coordinates and masses of the particle i, respectively.

Let us introduce the total three-body wave function as

a sum of two components [4]

$$\Psi(\vec{r}_1,\vec{r}_2,\vec{r}_3) \;=\; \Psi_1(\vec{r}_{23},\vec{\rho}_1) \;+\; \Psi_2(\vec{r}_{13},\vec{\rho}_2) \qquad (0.2)$$

where $\Psi_1(\vec{r}_{23},\vec{\rho}_1)$ is quadratically integrable over the variable $\vec{r}_{23}$, and $\Psi_2(\vec{r}_{13},\vec{\rho}_2)$ over $\vec{r}_{13}$. The components Ψ_1 and Ψ_2 carry the asymptotic boundary condition for channels 1 and 2, respectively. The second component is responsible for pure Coulomb interaction in the final state. These components satisfy the following set of two coupled equations [6]

$$\begin{aligned}[E \;-\; (H_0 + V_{23}(\vec{r}_{23}))]\Psi_1(\vec{r}_{23},\vec{\rho}_1) \\ = \;[(V_{23}(\vec{r}_{23}) + V_{12}(\vec{r}_{12})) - U_C(\vec{\rho}_2)]\Psi_2(\vec{r}_{13},\vec{\rho}_2)\end{aligned} \qquad (0.3)$$

$$\begin{aligned}[E \;-\; (H_0 + V_{13}(\vec{r}_{13})) -\; U_C\;(\vec{\rho}_2)]\Psi_2(\vec{r}_{13},\vec{\rho}_2) \\ = \;[(V_{13}(\vec{r}_{13}) + V_{12}(\vec{r}_{12}))]\Psi_1(\vec{r}_{23},\vec{\rho}_1)\end{aligned} \qquad (0.4)$$

where E is the center-of-mass energy, H_0 the total kinetic energy operator, $V_{ij}(\vec{r}_{ij})$ the pair potential ($i \neq j = 1,2,3$), U_C the final-state Coulomb interaction. For both $U_C = 0$ and $U_C \neq 0$, Eqs. 0.3 and 0.4 are equivalent to the underlying Schrödinger equation for the problem. Hence a converged solution of these equations should lead to the true dynamical solution of the problem. However, an approximate (low-order) close-coupling solution of these equations with the proper final-state Coulomb interaction U_C should lead to a more converged solution when compared with a similar solution with $U_C = 0$ as we shall see in the following. At higher energies the effect of the explicit inclusion of the Coulomb potential U_c in the equations above is reduced and the transfer rates for $U_c = 0$ tends towards those for $U_c \neq 0$.

We solve the integro-differential form of the Faddeev-Hahn equation by the close-coupling approximation scheme involving up to six states. This procedure consists in expanding the wave function components Ψ_1 and Ψ_2 in terms of eigenfunctions of subsystem Hamiltonians in initial and final channels, respectively. Although, these subsystem eigenfunctions are not orthogonal to each other, the components Ψ_1 and Ψ_2 satisfy a coupled set of equations incorporating the correct asymptotic behavior of the wave function. Consequently, there is no problem of overcompleteness as encountered in similar expansion approaches for rearrangement reactions based on the Schrödinger equation. The resultant coupled Faddeev-Hahn-type equations are then projected on the expansion functions. After a partial-wave projection this leads to a set of one-dimensional coupled integro-differential equations for the expansion coefficients, which is solved numerically. The mathematical details of the approach have appeared elsewhere and we refer the interested readers to the original references [2, 5].

First, we restrict ourselves to a two-level approximation by choosing in the relevant close-coupling expansion the hydrogen-like ground states $(H_\mu)_{1s}$ and $(He_\mu)^+_{1s}$, where H = $^1H^+$ and $^2H^+$, and He = $^3He^{++}$ and $^4He^{++}$. Numerically, stable and converged results were obtained in these cases. The rates $\lambda_{\rm tr}$ /10^6 sec^{-1} for both $U_C = 0$ and $U_C \neq 0$ at low energies are presented in Table I together with the results of Refs. [13, 14, 15]. Next we extend the calculation to the six-state model where we include the H_μ(1s,2s,2p) and $(He_\mu)^+$(1s,2s,2p) states of both muonic hydrogen and helium. These transition rates for both $U_C = 0$ and $U_C \neq 0$ are also shown in Table I. All rates have converged to the precision shown in this table. The present results are consistent with the phenomenological isotope effect, e.g., the rate decreases from ^{1}H to ^{2}H [12]. The effect of including the (2s,2p) states in the calculational scheme is also explicit.

The present six-state calculation, when compared with the two-state calculation, shows the trend of convergence. We see that at high energies the $U_c \neq 0$ rates tend towards the $U_c = 0$ rates. This is illustrated in Table I for the two-state model for two systems. However, the effect of the inclusion of U_c is significant at low energies. The two-state rates with $U_c = 0$ are the least converged. The six-state rates with $U_c = 0$ show the direction of convergence. From an analysis of our results reported in Table I, we find, as expected, the six-state results with $U_c \neq 0$ are the most converged. The two-state rates with $U_c \neq 0$ are more converged than the three-state rates with $U_c = 0$. The explicit inclusion of the final-state Coulomb interaction U_C has enhanced the convergence and has led to more consistent rates. The present six-state results for $U_C \neq 0$ are very close to the semiclassical results of Ref. [13] for all four systems considered. However, the agreement with the results of Ref. [14] is poor; the present rates for $^1H_\mu$ ($^2H_\mu$) are roughly double (ten times) the rates of Ref. [14]. Considering the very qualitative and semiclassical nature of the calculation of Ref. [15], the fair agreement with the present few-body quantum treatment and with Ref. [13] is encouraging.

The study of three-body charge transfer reactions with Coulomb repulsion in the final state has been the subject of this report. We have studied such reactions employing a detailed few-body description of the rearrangement scattering problem by solving the Faddeev-Hahn-type equations [3, 4] in coordinate space. To provide correct asymptotic form in the final state the pure Coulomb interaction has been incorporated directly into the equations. It is shown that within this formalism, the application of a close-coupling-type ansatz leads to satisfactory results already in low-order approximations for direct muon-transfer reactions between hydrogen isotopes and light nuclei He^{++}. Because of computational difficulties, in this application we have considered up to six states in the expansion scheme (1s,2s,2p on each center – H_μ and He^+_μ), which may not always be adequate. Further calculations with larger basis sets are needed to obtain accurate converged results. However, the inclusion of three basis states on each center is expected to build in a satisfactory account of the polarization potential in the model and should lead to physically acceptable results. The agreement of the present rates with those of the semiclassical model also assuring.

Acknowledgments

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Table I. Low-energy muon-transfer rates $\lambda_{\rm tr}/10^6$ sec^{-1} from proton $(^1{\rm H}_\mu)_{1s}$ and deuteron $(^2{\rm H}_\mu)_{1s}$ to hydrogen-like ground states $(^3{\rm He}_\mu)^+_{1s}$ and $(^4{\rm He}_\mu)^+_{1s}$ within six-state close-coupling model.

System	Energy	Two-state result		Six-state result		Other result
	(eV)	$U_c=0$	$U_c\neq 0$	$U_c=0$	$U_c\neq 0$	
$^1{\rm H}_\mu+{}^3{\rm He}^{++}$	0.001	2.1	8.4	3.8	13.6	
	0.01	2.1	8.4	3.4	13.3	
	0.04	2.1	8.4	3.3	12.5	10.9[13],6.3[14],7.25[15]
	0.1	2.0	8.3	3.2	11.0	
	5	1.4	5.6			
	60	0.5	1.0			
$^2{\rm H}_\mu+{}^3{\rm He}^{++}$	0.001	1.3	5.2	2.8	9.7	
	0.01	1.3	5.2	2.7	9.5	
	0.04	1.3	5.2	2.6	9.4	9.6[13], 1.3[14], 4.77[15]
	0.1	1.2	5.1	2.3	8.8	
	5	0.6	3.2			
	60	0.1	0.15			
$^1{\rm H}_\mu+{}^4{\rm He}^{++}$	0.001	1.4	6.8	3.2	12.8	
	0.01	1.4	6.8	2.8	12.4	
	0.04	1.4	6.8	2.6	11.8	10.7[13],5.5[14],6.65[15]
	0.1	1.3	6.7	2.3	10.6	
$^2{\rm H}_\mu+{}^4{\rm He}^{++}$	0.001	0.8	5.0	1.7	9.6	
	0.01	0.8	5.0	1.6	9.5	
	0.04	0.8	5.0	1.6	9.3	9.6[13],1.0[14],4.17[15]
	0.1	0.8	4.9	1.2	8.8	